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Global sensitivity analysis using sparse grid interpolation and polynomial chaos ☆

Gregery T. Buzzard *

Department of Mathematics, Purdue University, West Lafayette, IN 47907, United States

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ABSTRACT

Sparse grid interpolation is widely used to provide good approximations to smooth functions in high dimensions based on relatively few function evaluations. By using an efficient conversion from the interpolating polynomial provided by evaluations on a sparse grid to a representation in terms of orthogonal polynomials (gPC representation), we show how to use these relatively few function evaluations to estimate several types of sensitivity coefficients and to provide estimates on local minima and maxima. First, we provide a good estimate of the variance-based sensitivity coefficients of Sobol' (1990) [1] and then use the gradient of the gPC representation to give good approximations to the derivative-based sensitivity coefficients described by Kucherenko and Sobol' (2009) [2]. Finally, we use the package HOM4PS-2.0 given in Lee et al. (2008) [3] to determine the critical points of the interpolating polynomial and use these to determine the local minima and maxima of this polynomial.
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1. Introduction

A common task in fitting a model to data is to find parameters $p=(p_1,\ldots,p_n)$ to minimize some cost function, $C(p)$, often a sum of squared differences between model output and experimental data. This is a particularly a difficult task when the dimensionality of the parameter space is large and the dependence of C on p is nonlinear. One approach to this problem is to sample the function at some set of points and try to estimate relevant quantities, such as various types of sensitivity coefficients and the location of local minima, from this sample. Often, these samples are used to construct a simpler model (e.g., linear, polynomial, sum of Gaussians, etc.) that may be used to approximate the original model in a computationally inexpensive way. Such approximate models are described with various terms, including metamodels, surrogate models, response surfaces and model emulators. In settings in which the sampling points are given in advance, common approaches include RS-HDMR, cut-HDMR, ANOVA decomposition, kriging, and moving least squares. In settings in which the sampling points may be chosen at will, two common approaches are sparse grid interpolation and generalized polynomial chaos (gPC) using cubature. In this paper we focus on these last two metamodels, the relationship between them, and their application to computing global sensitivity coefficients and global maxima and minima.

More precisely, sensitivity methods can be divided into global (the focus in this paper) and local, while global methods can in turn be divided into screening methods, non-parametric methods, variance-based methods, and moment-independent or density based methods. The classic paper on screening methods is [4], which details a method for sampling model outputs over a high-dimensional input space in order to estimate the mean and variance of partial derivatives of the output with respect to each input. A number of non-parametric approaches for global SA, including locally weighted regression, additive models, projection pursuit regression, and recursive partitioning regression are detailed in [5]. Further non-parametric methods, along with a description for using these methods to estimate values and confidence intervals for variance-based sensitivity coefficients are given in [6]. An overview of global SA methods is provided in [7], which also introduces a new, moment-independent importance measure; this measure is discussed also in [8]. Many global SA methods are discussed in [9]. In terms of other metamodels, an overview of Kriging and discussion of bootstrapping to estimate the variance in the Kriging predictor is given in [10]. A discussion of gPC and its application to computing sensitivity coefficients appears in both [11,12].

Another approach to constructing a polynomial metamodel is sparse grid interpolation, which has been used widely in recent years as a means of providing a reasonable approximation to a smooth function, f, defined on a hypercube in $\mathbb{R}^n$, based on relatively few function evaluations [13]. This method produces a polynomial

Abbreviations: gPC, generalized polynomial chaos; MC, Monte Carlo; CGL, Chebyshev–Gauss–Lobatto

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* Tel.: +1 765 494 1937; fax: +1 765 494 0548.
E-mail addresses: buzzard@math.purdue.edu, greg.buzzard@gmail.com

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interpolant using Lagrange interpolating polynomials based on function values at points in a union of product grids of small dimension [14,15]. However, for many purposes, there are computational advantages to a representation in terms of orthogonal polynomials; such a representation is also known as a generalized polynomial chaos (gPC) representation. Most relevant for the discussion here is the efficient calculation of the Sobol' sensitivity coefficients of a polynomial in gPC form.

In this paper we start with the efficient conversion from an interpolating polynomial in Lagrange form to the gPC form as described in [16]. We combine this with the efficient calculation of the Sobol' sensitivity coefficients of [12,11] to produce an efficient algorithm for estimating these coefficients using a relatively small number of function evaluations. As seen in numerical examples, this method is both accurate and efficient for smooth functions when compared with other approaches for estimating these values. We also show how to use the gPC representation to estimate two derivative-based sensitivity measures discussed in [2]. Finally, we discuss the use of polynomial homotopy methods for finding the critical points of the interpolating polynomial [3]. In cases in which the global maximum or minimum does not lie on the boundary of the interpolating hypercube, this allows us to find the global minimum or maximum (within the hypercube) directly. In addition to these applications, we note that sparse grid interpolation likely has applications in the context of other global SA methods as well. We leave this as a topic for future research.

2. Theory

In this section we provide further background on sparse grid interpolation, generalized polynomial chaos, and sensitivity analysis.

2.1. Sparse grid interpolation and polynomial chaos

In one variable, Lagrange interpolation proceeds by selecting a set of points, $x_1,\ldots,x_n$ and degree $n-1$ polynomials L_j so that L_j is 1 at x_j and 0 at x_k for $k\neq j$. Given function values $f(x_j)$, we obtain an interpolating polynomial that agrees with f at each x_j by taking $P(x)=\sum_{j=1}^{n} f(x_j)L_j(x)$. For a well-chosen set of points, such as the Chebyshev–Gauss–Lobatto (CGL) points, and for smooth f, the resulting polynomials converge to f quite rapidly as the number of interpolating points is increased [14]. The simplest generalization of this to d dimensions is to use a full product grid obtained from the product of d one-dimensional interpolating sets, with Lagrange polynomials obtained by taking products of the one-dimensional Lagrange polynomials. However, since the resulting number of points is exponential in d, this method is not practical for anything but small d. As described in [14] and elsewhere, Smolyak [15] devised a method in which the interpolating points in a hypercube, $[0,1]^d$, in d dimensions are obtained as a union of smaller product grids. Examples of full and sparse grids in two dimensions appear in Fig. 1.

In the sparse grid, the dotted points show the locations of all the points in the sparse grid, while the circled points show the points in one product subgrid. This example shows that using sparse grid points, the function is sampled heavily along the coordinate axes, then somewhat less near corners and boundaries, and even less in the interior. With these values, we can again represent f as a sum of products of one variable Lagrange polynomials. On each of the smaller product grids in the sparse grid, this is a simple tensorization of the one-dimensional Lagrange representation given above. The contributions for different subgrids are then summed with appropriate weights to produce the interpolating polynomial on the entire sparse grid. The use of a nested sequence of points in one dimension, such as appropriate subsets of CGL points, implies that the good convergence properties of interpolation in one dimension carry over to higher dimensions. Details of the sparse grid construction and precise estimates on the rate of convergence may be found in [14]. With appropriate modifications, sparse grid interpolation may also be performed on hypercubes in which some of the sides are unbounded [16].

In the gPC representation of f, the function is still represented as the sum of products of polynomials in one variable, but now the underlying one dimensional polynomials are orthogonal in the weighted L^2 sense. That is, over some fixed interval, I, in the real line, and with some fixed positive weight function $w(x)$, they satisfy $\int_I P_j(x)P_k(x)w(x)\,dx=\delta_{jk}$. A common example is the Legendre polynomials, which are orthogonal over the interval $[-1,1]$ using the weight function $w(x)=1$. The weight function often corresponds to a probability distribution. More details may be found in [13,12].

2.2. Sensitivity analysis

As described in [1,17] and elsewhere, a useful decomposition of a function $f(x)=f(x_1,\ldots,x_n)$ defined on a hypercube in $\mathbb{R}^n$ is to write it as a normalized sum of functions that depend on a specified subset of the variables:

$$f(x)=f_0+\sum_{i=1}^{n} f_i(x_i)+\sum_{1\le i<j\le n} f_{ij}(x_i,x_j)+\cdots+f_{12\ldots n}(x_1,\ldots,x_n),$$

with a (weighted) orthogonality condition imposed on pairs of functions in this decomposition and a 0 mean condition in each variable separately imposed on each function individually. In various contexts this decomposition is known as the Sobol' decomposition, the ANOVA decomposition, or the HDMR representation of f. As described in [17,12], one method for achieving this decomposition is by expanding f in terms of a basis of tensored one-dimensional

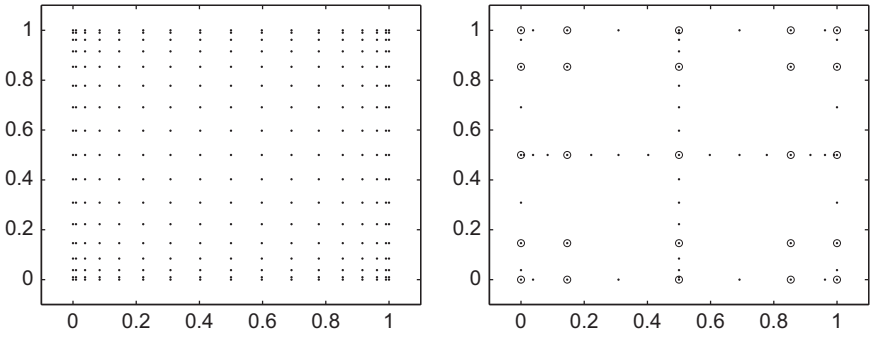

Fig. 1. Full and sparse grids in two dimensions using CGL points. Left: The full grid is obtained as a product of the points along the coordinate axes in the sparse grid. Right: The dotted points show the entire sparse grid of nesting depth 4, while the circled points show one of the component product subgrids.

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